

chain nodes :

7 8 9 10 11 12 13 14 15 18 19 20 21 22

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 6-18 7-8 7-9 9-10 10-11 11-12 11-13 14-15 18-22 19-20 19-22 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8 7-9 9-10 11-12 11-13 14-15 18-22 19-20 19-22 20-21

exact bonds :

5-7 6-18 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:H,[*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS12:CLASS13:CLASS14:CLASS15:CLASS18:CLASS19:CLASS20:CLASS21:Atom 22:CLASS

Generic attributes :

21:

Saturation : Unsaturated

Number of Carbon Atoms : 7 or more

Type of Ring System : Polycyclic

Element Count :

Node 21: Limited

N,N1

O,O0

S,S0

10/690400

=>

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chain nodes :

7 8 9 10 11 12 13 14 15 18 19 20 21 22

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 6-18 7-8 7-9 9-10 10-11 11-12 11-13 14-15 18-22 19-20 19-22 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8 7-9 9-10 11-12 11-13 14-15 18-22 19-20 19-22 20-21

exact bonds :

5-7 6-18 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:H, [*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS 19:CLASS 20:CLASS

21:Atom 22:CLASS

Generic attributes :

21:

10/690400

Saturation : Unsaturated
Number of Carbon Atoms : 7 or more
Type of Ring System : Polycyclic

Element Count :
Node 21: Limited

N,N1
O,OO
S,SO

L1 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 13:51:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2574 TO ITERATE

77.7% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 48437 TO 54523
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 13:51:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 50851 TO ITERATE

100.0% PROCESSED 50851 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.02

L3 4 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
172.55 172.76

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17:

Saturation : Unsaturated
Number of Carbon Atoms : less than 7

Element Count :

Node 17: Limited

N, NO-1

O, OO

S, SO

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FILE COVERS 1907 - 29 May 2007 VOL 146 ISS 23
 FILE LAST UPDATED: 28 May 2007 (20070528/ED)

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 They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13
 L4 3 L3

=> d 14 1-3 bib abs hitstr

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 1999:764022 CAPLUS
 DN 132:3323
 TI Preparation of tetrahydroisoquinolinylnicotinic acid amides and related compounds as inhibitors of cysteine proteases.
 IN Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika
 PA BASF Aktiengesellschaft, Germany
 SO PCT Int. Appl., 57 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9961423	A1	19991202	WO 1999-EP3549	19990525
	W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, ZA, AM, AZ, KG, MD, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2333008	A1	19991202	CA 1999-2333008	19990525
	AU 9945003	A	19991213	AU 1999-45003	19990525
	BR 9910701	A	20010130	BR 1999-10701	19990525
	EP 1080074	A1	20010307	EP 1999-927749	19990525
	EP 1080074	B1	20061108		
	R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE, FI				
	HU 200102146	A2	20011128	HU 2001-2146	19990525
	JP 2002516311	T	20020604	JP 2000-550829	19990525
	AT 344794	T	20061115	AT 1999-927749	19990525
	EP 1757584	A1	20070228	EP 2006-23149	19990525
	R: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE, AL, LT, LV, MK, RO, SI				
	US 6482832	B1	20021119	US 2000-700453	20001115
	NO 2000005929	A	20001123	NO 2000-5929	20001123
	ZA 2000007757	A	20020121	ZA 2000-7757	20001221
PRAI	DE 1998-19823245	A	19980525		
	EP 1999-927749	A3	19990525		
	WO 1999-EP3549	W	19990525		
OS	MARPAT 132:3323				
AB	AB(R1)nCONHCHR2COR3 [A = (substituted) tetrahydro(iso)quinoliny, dihydro(iso)indolyl; B = Ph, naphthyl, pyridyl, pyrimidinyl, quinolyl, thieryl, furyl, etc.; R1 = H, alkyl, alkoxy, alkenyl, alkynyl, alkylphenyl, OH, Cl, F, Br, iodo, etc.; n = 0-2; R2 = (substituted) alkyl; R3 = H, CO2R5, COZ; Z = (substituted) amino, piperazinyl, pyrrolidinyl, piperidinyl; R5 = (substituted) alkyl], were prepared Thus, Et				

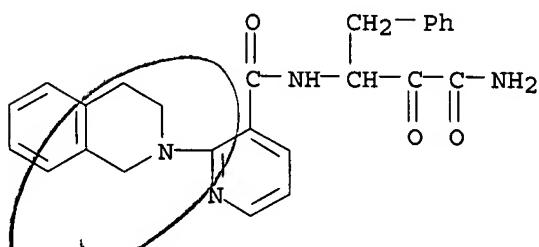
2-chloronicotinate, 1,2,3,4-tetrahydroisoquinoline hydrochloride, and K₂CO₃ were heated in DMF at 110° to give 87% Et 2-(1,2,3,4-tetrahydroisoquinolin-2-yl)nicotinate. This was saponified with aqueous NaOH in EtOH (81%) and the product was stirred with 3-amino-2-hydroxy-4-phenylbutyramide hydrochloride, Et₃N, 1-hydroxybenzotriazole, and N'-3-dimethylaminopropyl-N-ethylcarbodiimide to give 85% 2-(1,2,3,4-tetrahydroisoquinolin-2-yl)nicotinic acid [N-(1-carbamoyl-1-hydroxy-3-phenylpropan-2-yl)]amide. The latter was stirred with pyridine-SO₃ in Me₂SO to give 31% 2-(1,2,3,4-tetrahydroisoquinolin-2-yl)nicotinic acid [N-(1-carbamoyl-1-oxo-3-phenylpropan-2-yl)]amide.

IT 247056-67-3P 247056-68-4P 250739-05-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of tetrahydroisoquinolinyl nicotinic acid amides and related compds. as inhibitors of cysteine proteases)

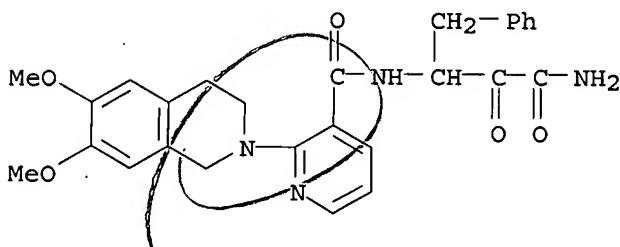
RN 247056-67-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



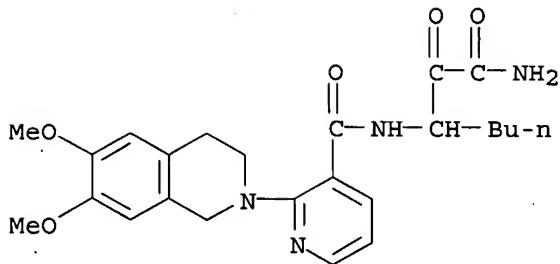
RN 247056-68-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



RN 250739-05-0 CAPLUS

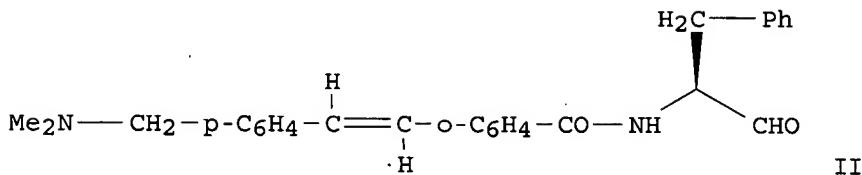
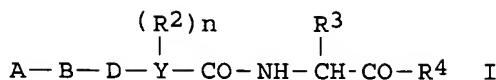
CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 1999:691085 CAPLUS
 DN 131:310835
 TI Preparation of cysteine protease inhibitors for therapeutic use
 IN Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika
 PA BASF Aktiengesellschaft, Germany
 SO PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9954310	A2	19991028	WO 1999-EP2633	19990420
	WO 9954310	A3	20000217		
	W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, ZA, AM, AZ, KG, MD, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2328396	A1	19991028	CA 1999-2328396	19990420
	AU 9939276	A	19991108	AU 1999-39276	19990420
	BR 9909774	A	20001219	BR 1999-9774	19990420
	EP 1073641	A2	20010207	EP 1999-922108	19990420
	EP 1073641	B1	20040414		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
	TR 200003068	T2	20010321	TR 2000-200003068	19990420
	HU 200102732	A2	20011228	HU 2001-2732	19990420
	JP 2002512231	T	20020423	JP 2000-544649	19990420
	AT 264310	T	20040415	AT 1999-922108	19990420
	ES 2220061	T3	20041201	ES 1999-922108	19990420
	US 6753327	B1	20040622	US 2000-673089	19990420
	BG 104873	A	20010731	BG 2000-104873	20001011
	NO 2000005263	A	20001019	NO 2000-5263	20001019
	IN 2000CN00655	A	20050304	IN 2000-CN655	20001113
	HR 2000000787	A1	20010831	HR 2000-787	20001117
	ZA 2000006719	A	20020815	ZA 2000-6719	20001117
	US 2004082569	A1	20040429	US 2003-690400	20031020
PRAI	DE 1998-19818615	A	19980420		
	WO 1999-EP2633	W	19990420		
	US 2000-673089	A3	20001011		
OS	MARPAT	131:310835			
GI					



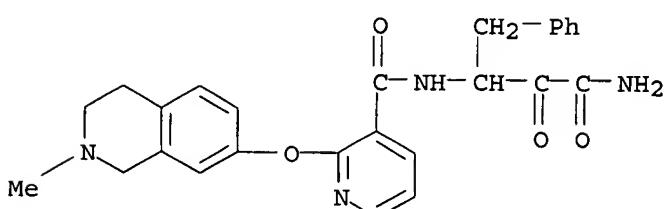
AB The invention relates to cysteine protease inhibitors of the general formula [(I); A = -(CH₂)_p-R₁; R₁ = pyrrolidine, morpholine, piperidine, -NR₅R₆, (N-substituted)piperazine; R₅, R₆ = independently H, alkyl, cyclohexyl, cyclopentyl, (CH₂)_nPh, where Ph may be R₆-substituted; p = 1-2; B = (substituted) Ph, pyridyl, pyrimidyl or pyridazyl; D = bond, -(CH₂)_m-, -CH:CH-, -C.tplbond.C-; R₂ = Cl, Br, F, alkyl, NHCO alkyl, NHSO₂ alkyl, NO₂, -O-alkyl or NH₂; R₃ = alkyl which can carry a (substituted) Ph ring, indolyl ring or cyclohexyl ring; Y = Ph, pyridine, pyrimidine or pyrazine; R₄ = H, COOR₉ or CO-Z, where Z = NR₁₀R₁₁; R₉, R₁₀, R₁₁ = (independently) H, (unsubstituted) (unbranched) alkyl; n = 0-2 and m = 0-4]. Thus, Et 2-bromo-benzoate and dimethyl(4-vinylbenzyl)amine were reacted, de-esterified, and the free acid intermediate reacted with (S)-phenylalaninol to give an intermediate which was reduced to give aldehyde (II) in 88% yield. Title compds. showed good results as inhibitors of calpain I and II or cathepsin B in a variety of in vivo and in vitro tests (no data given).

IT 247219-18-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of as cysteine protease inhibitors for therapeutic use)

RN 247219-18-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[(1,2,3,4-tetrahydro-2-methyl-7-isoquinolinyl)oxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:684297 CAPLUS

DN 131:299438

TI New substituted heterocyclic amides, their preparation and application

IN Lubisch, Wilfried; Moeller, Achim; Treiber, Hans-Joerg; Knopp, Monika

PA BASF A.-G., Germany

SO Ger. Offen., 36 pp.

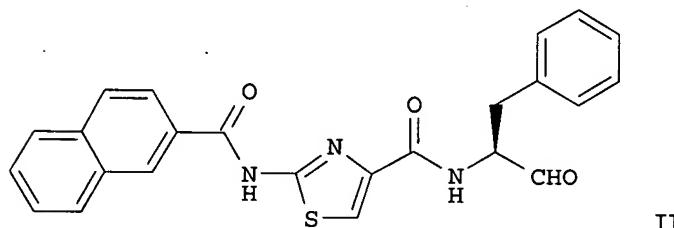
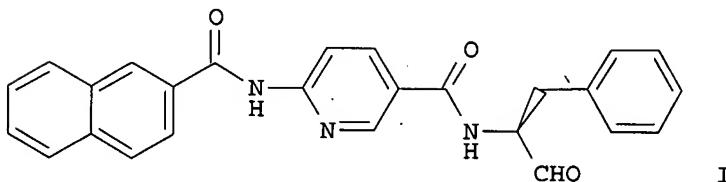
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19817459	A1	19991021	DE 1998-19817459	19980420
	CA 2328438	A1	19991028	CA 1999-2328438	19990419
	WO 9954304	A1	19991028	WO 1999-EP2611	19990419
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9939271	A	19991108	AU 1999-39271	19990419
	BR 9909772	A	20001219	BR 1999-9772	19990419
	EP 1073638	A1	20010207	EP 1999-922102	19990419
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
	TR 200003056	T2	20010221	TR 2000-200003056	19990419
	HU 200101688	A2	20011128	HU 2001-1688	19990419
	JP 2002512228	T	20020423	JP 2000-544645	19990419
	BG 104831	A	20010531	BG 2000-104831	20001010
	US 6630493	B1	20031007	US 2000-673087	20001011
	NO 2000005264	A	20001019	NO 2000-5264	20001019
	HR 2000000786	A1	20010831	HR 2000-786	20001117
	ZA 2000006718	A	20011119	ZA 2000-6718	20001117
	US 2004097508	A1	20040520	US 2003-601356	20030623
PRAI	DE 1998-19817459	A	19980420		
	WO 1999-EP2611	W	19990419		
	US 2000-673087	A3	20001011		
OS	MARPAT 131:299438				
GI					



AB Heterocyclic amides such as I and II were prepared as inhibitors of enzymes, e.g., calpains and cathepsin B. Thus, II was prepared in 4 steps starting from Et 2-amino-4-thiazolecarboxylate and 2-naphthoyl chloride.

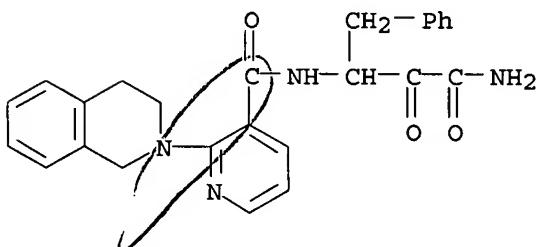
IT 247056-67-3P 247056-68-4P

10/690400

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(heterocyclic amides as enzyme inhibitors)

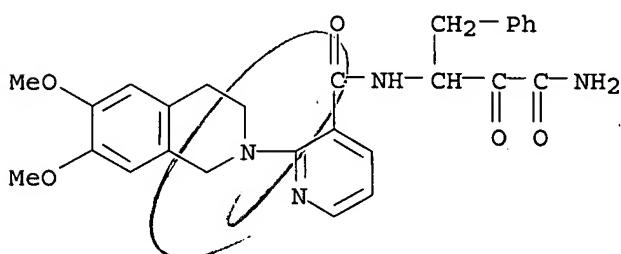
RN 247056-67-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



RN 247056-68-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST

18.63	191.39
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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10/690400

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=> s 13
L5 0 L3

=> log h
COST IN U.S. DOLLARS

FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	191.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

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STN INTERNATIONAL SESSION SUSPENDED AT 13:55:36 ON 29 MAY 2007